Reentrant superconductivity in a strong applied field within the tight–binding model

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It was suggested by Rasolt and Tešanović that the Landau level quantization in isotropic superconductors could enhance superconductivity in a very strong magnetic field, above the upper critical field (H_{c2}). We derive a generalized Harper equation for superconducting systems, and show that a similar reentrant behavior appears in a lattice model, even though the Landau–level–structure is destroyed by the periodic potential in that case. Both the orbital and the Zeeman field–induced effects are taken into account.

I. INTRODUCTION

There are two mechanisms responsible for a suppression of conventional superconductivity in an external magnetic field[1]: the Pauli pair breaking and the diamagnetic pair breaking. First of them, the Pauli pair breaking, is connected with the Zeeman coupling. The magnetic field tends to align the spins of the electrons forming the Cooper pair, and the singlet superconductivity disappears at the Chandrasekhar–Clogston (CC) limit[2]. However, this critical field for the majority of type–II systems is found to be above H_{c2} determined by the orbital (diamagnetic) pair–breaking. Especially, this effect is of minor significance in materials with low effective g–factor. Another possibility is the superconductivity with nonhomogeneous order parameter (the Larkin–Ovchinnikov–Fulde–Ferrell state[3]), which can exist above the CC limit. One can also look for high–magnetic–field superconductivity in superconductors with triplet equal spin pairing.

The second effect, the diamagnetic pair–breaking, usually crucial in determining the upper critical field, is connected with the orbital frustration of the superconducting order parameter in a magnetic field. This frustration enlarges the free energy of the superconducting state, and, when the magnetic field is strong enough, the normal state becomes energetically favorable. The orbital effect can be reduced in layered two–dimensional superconductors, when the applied magnetic field is parallel to the conducting layers. Such a situation has been analyzed theoretically[4] and recently observed experimentally in organic conductors[5].

However, it was shown that large values of the critical field are possible also in the systems without two–dimensional layers, i.e., in systems where the orbital effects are present. When describing a superconductor within the Ginzburg–Landau-Abrikosov–Gor'kov theory[6], one treats the magnetic field in the semiclassical phase–integral approximation, thus neglecting the quantum effects of the magnetic field. This approximation is valid for relatively small fields, when $\hbar\omega_c \ll k_B T_c$ (or $\omega_c \ll 2\pi/\tau$ for large impurity concentration, where τ is the elastic scattering time). In this regime, the number of occupied Landau levels is very large and the energy spacing of them is very small, and therefore this discrete structure is not observable. However, when the magnetic field increases, the Landau-level degeneracy also increases, so the number of occupied levels decreases and one has to take it into account. The inclusion of the Landau level quantization in the BCS theory leads to reentrant behavior at a very high magnetic field ($\hbar\omega_c \gg \epsilon_F$). Namely, when only the lowest Landau level is occupied, T_c is increasing function of H, limited only by impurity scattering and the Pauli pair breaking effect.

The aim of this paper is to show that the reentrant behavior survives in the presence of a strong periodic lattice potential.

Weak, unidirectional periodic potential removes (or, at least, modify) the Landau–level structure: the levels are broadened (they form "Landau bands") and the degeneracy is lifted[7]. The width of a Landau band oscillates as the magnetic field is tuned as a consequence of commensurability between the cyclotron diameter and the period of the potential. It results in a magnetoresistance oscillations (Weiss oscillations[8]). If the periodic potential is modulated in two dimensions, "minigaps" open in the "Landau bands", and the energy spectrum of the system plotted versus the applied field composes the famous Hofstadter butterfly[7,9], recently observed experimentally in the quantized–Hall–conductance measurement[10]. The same spectrum can be obtained in a complementary limit, when the lattice potential is strong (tight binding approach) and the field is weak. It is interesting that when the periodic potential does not lead to a scattering between states from different Landau levels, the eigenvalue equations in both the limiting cases are formally the same[7]. Of course the parameters have a different physical meaning.

The simplest model for the case where a aplied field and a lattice potential are present simultaneously, is commonly referred to as the Hofstadter or Azbel–Hofstadter model[9,11]. The corresponding Hamiltonian describes electrons on a two–dimensional square lattice with the nearest–neighbor hopping, in a perpendicular uniform magnetic field. The Schrödinger equation takes the form of a one–dimensional difference equation, known as the Harper equation (or the almost Mathieu equation)[9,12,13]. It is also a model for one–dimensional electronic system in two incommensurate periodic potentials. The Harper equation has also links to many other areas of

interest, e.g., the quantum Hall effect, quasicrystals, localization–delocalization phenomena[14,15], the noncommutative geometry[16], the renormalization group[17,18], the theory of fractals, the number theory, and the functional analysis[19].

The Hofstadter model is useful in approach to the fundamental problem of the external magnetic field influence on the superconductivity. Most of the works devoted to superconductors in the mixed state are based on the Bogolubov–de Gennes equations[20], particularly useful for spatially inhomogeneous systems, e.g., for an isolated vortex[21] or a vortex lattice[22]. However, in the regime $H_{c1} \ll H \ll H_{c2}$ we can neglect contributions to the spectrum from the inside of the vortex core (for $H \ll H_{c2}$ the distance between the vortices is large) and regard the magnetic field as uniform in the sample (for $H_{c1} \ll H$). We derive, under these assumptions, a lattice model for the superconductor in applied field (in the normal state such a system is described by the Hofstadter model). In this paper we present a generalized Harper equation that describes the influence of magnetic field on the two–dimensional tightly bound electrons in the superconducting state.

II. THE MODEL

In analogy to Hofstadter's approach, we couple the magnetic field to the system via the Peierls substitution[23], i.e., multiply the hopping matrix elements by a phase factor which depends on the field and on the position within the lattice. Thus, the vector–potential–dependent hopping integral for sites i and j is given by

$$t_{ij}\left(\mathbf{A}\right) = t \exp\left(\frac{ie}{\hbar c}\int_{\mathbf{R}_j}^{\mathbf{R}_i} \mathbf{A}\cdot d\mathbf{l}\right), \tag{1}$$

where t is the usual hopping integral. We also include the Zeeman term. In effect, the BCS Hamiltonian has the form

$$\begin{aligned}\hat{H} &= \sum_{\langle ij\rangle,\sigma} t_{ij}\left(\mathbf{A}\right) c^{\dagger}_{i\sigma}c_{j\sigma} + \sum_{i,\sigma}\left(\epsilon_\sigma - \mu\right) c^{\dagger}_{i\sigma}c_{i\sigma} \\ &\quad - \sum_{\langle ij\rangle}\left(\Delta_{ij} c^{\dagger}_{i\uparrow}c^{\dagger}_{j\downarrow} + \Delta^{*}_{ij} c_{i\downarrow}c_{j\uparrow}\right),\end{aligned} \tag{2}$$

where the Zeeman splitting is given by $\epsilon_\sigma = -\frac{1}{2}\sigma g\mu_B H$, $\sigma = 1$ for spin up and -1 for spin down, g is the Landé factor, and μ is the chemical potential. Here, we have introduced the spin–singlet pair amplitude $\Delta_{ij} = \frac{V}{2}\langle c_{i\uparrow}c_{j\downarrow} - c_{i\downarrow}c_{j\uparrow}\rangle$. The strength of the nearest neighbor attraction V is assumed to be field independent. The validity of this assumption depends on the nature of pairing potential and the strength of the magnetic field.[24] For example, in the $t-J$ model $J_{ij}(\mathbf{A}) = 4t_{ij}(\mathbf{A})t_{ji}(\mathbf{A})/U$ is strictly field independent, since the change of the phase generated when an electron hops from site i to j and back, cancels out. Such an assumption has been also partially justified on the basis of antiferromagnetic–spin–fluctuation–driven superconductivity.[25]

Our starting point is a two–dimensional square lattice with basis vectors $\mathbf{a} = (a,0,0)$ and $\mathbf{b} = (0,a,0)$, immersed in a perpendicular, uniform magnetic field $\mathbf{H} = (0,0,H)$. We choose the Landau gauge, $\mathbf{A} = (0,Hx,0)$. Since the vector potential $\mathbf{A}$ is linear in x, the translation corresponding to the vector $\mathbf{a}$ shifts the phase of the wave function. This shift can be compensated by a gauge transformation, introducing *magnetic translations*. If the magnetic flux per unit cell, Φ, is a rational multiple of the flux quantum $\Phi_0 = hc/e$, i.e., if

$$\frac{\Phi}{\Phi_0} = \frac{p}{q}, \tag{3}$$

with p and q coprime integers, we can define *magnetic lattice*, with $q\mathbf{a}$ and $\mathbf{b}$ as the basis of the *magnetic unit cell*. Such an enlarged unit cell is penetrated by p flux quanta. Magnetic translations corresponding to the *magnetic lattice* vectors ($\mathbf{R} = nq\mathbf{a}+m\mathbf{b}$, with n,m – integers) commute with each other and with the Hamiltonian. If the system is of rectangular shape with L_x sites in the x direction and L_y sites in the y direction, and L_x is a multiple of q, we can find eigenfunctions which diagonalize the Hamiltonian and the magnetic translation operators simultaneously. Due to the absence of translational invariance with vectors $m\mathbf{b}$, vectors $\mathbf{k} = (k_x,\ k_y)$ from the firs Brillouin zone ($|k_x| \le \pi/a,\ |k_y| \le \pi/a$) are not good quantum numbers. Instead, we have to use vectors from a *magnetic (reduced) Brillouin zone* (MBZ), defined by $|k_x| \le \pi/qa,\ |k_y| \le \pi/a$, to enumerate the eigenstates. The Hamiltonian (1) in the momentum space can be written as

$$\begin{aligned}\hat{H} &= -t\sum_{\mathbf{k},\sigma}\Big[2\,\cos\left(k_x a\right) c^{\dagger}_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma} \\ &\quad + e^{-ik_y a}c^{\dagger}_{\mathbf{k}-\mathbf{g},\sigma}c_{\mathbf{k},\sigma} + e^{ik_y a}c^{\dagger}_{\mathbf{k}+\mathbf{g},\sigma}c_{\mathbf{k},\sigma}\Big] \\ &\quad + \sum_{\mathbf{k}\sigma}\left(\epsilon_\sigma - \mu\right) c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} - \sum_{\mathbf{k}}\left(\Delta_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{-\mathbf{k}\downarrow} + \mathrm{H.c.}\right),\end{aligned} \tag{4}$$

where

$$\Delta_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\langle c_{-\mathbf{k}'\downarrow}c_{\mathbf{k}'\uparrow}\rangle, \tag{5}$$

and $\mathbf{g} = (2\pi p/q, 0)$. In order to rewrite the above Hamiltonian as a sum over the MBZ we introduce a multicomponent Nambu spinors

$$\begin{aligned}C^{\dagger}_{\mathbf{k}} &= \Big(c^{\dagger}_{\mathbf{k},\uparrow},\ c^{\dagger}_{\mathbf{k}-\mathbf{g},\uparrow},\ c^{\dagger}_{\mathbf{k}-2\mathbf{g},\uparrow},\ \ldots,\ c^{\dagger}_{\mathbf{k}-(q-1)\mathbf{g},\uparrow}, \\ &\quad c_{-\mathbf{k},\downarrow},\ c_{-\mathbf{k}+\mathbf{g},\downarrow},\ c_{-\mathbf{k}+2\mathbf{g},\downarrow},\ \ldots,\ c_{-\mathbf{k}+(q-1)\mathbf{g},\downarrow}\Big)\end{aligned} \tag{6}$$

Then Eq. (4) can be written as

$$\hat{H} = {\sum_{\mathbf{k}}}' C^{\dagger}_{\mathbf{k}} H_{\mathbf{k}} C_{\mathbf{k}}, \tag{7}$$

where the prime denotes summation over the MBZ and $H_{\mathbf{k}}$ has a block structure

$$H_{\mathbf{k}} = \left(\begin{array}{c|c} \hat{\mathbf{T}}_{\mathbf{k}\uparrow} & \hat{\mathbf{\Delta}}_{\mathbf{k}} \\ \hline \hat{\mathbf{\Delta}}^*_{\mathbf{k}} & -\hat{\mathbf{T}}_{-\mathbf{k}\downarrow} \end{array} \right). \tag{8}$$

The diagonal blocks describe noninteracting lattice fermions under the influence of magnetic field, and have the form similar to that derived by Hasegawa *et al.*[26]

$$\hat{\mathbf{T}}_{\mathbf{k},\sigma} = -t \begin{pmatrix} M_{0,\sigma} & e^{ik_y} & 0 & \cdots & 0 & e^{-ik_y} \\ e^{-ik_y} & M_{1,\sigma} & e^{ik_y} & 0 & \cdots & 0 \\ 0 & e^{-ik_y} & M_{2,\sigma} & e^{ik_y} & \cdots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \vdots & 0 & e^{-ik_y} & M_{q-2,\sigma} & e^{ik_y} \\ e^{ik_y} & 0 & \vdots & 0 & e^{-ik_y} & M_{q-1,\sigma} \end{pmatrix}, \tag{9}$$

where $M_{n,\sigma} = 2\cos(k_x a + n\gamma) + \epsilon_\sigma - \mu$, $\gamma = |\mathbf{g}| = 2\pi p/q$, and diagonal matrix $\hat{\mathbf{\Delta}}_{\mathbf{k}}$ represents the pairing amplitudes

$$\hat{\mathbf{\Delta}}_{\mathbf{k}} = \mathrm{diag}\left(\Delta_{\mathbf{k}},\, \Delta_{\mathbf{k}-\mathbf{g}},\, \ldots,\, \Delta_{\mathbf{k}-(q-1)\mathbf{g}}\right). \tag{10}$$

Diagonalization of Eq. (8) provides a set of eigenenergies $\{\mathcal{E}_{\mathbf{k},i}\}$, where i enumerates $2q$ values corresponding to a given $\mathbf{k}$ from the MBZ.

The pairing amplitude in the presence of external magnetic field is determined self–consistently from the BCS–like equation

$$\Delta_{\mathbf{k}} = \frac{1}{2N} {\sum_{\mathbf{k}'}}' \sum_{i=1}^{2q} \frac{V_{\mathbf{k},\mathbf{k}'}\Delta_{\mathbf{k}'}}{2\mathcal{E}_{\mathbf{k}',i}} \tanh\frac{\mathcal{E}_{\mathbf{k}',i}}{2k_B T}, \tag{11}$$

where $N = L_x L_y$ and the prime summation denotes again summation over the MBZ. In the following we restrict ourselves to the singlet pairing in the s–wave channel ($\Delta_{\mathbf{k}} = \Delta$), even though Eq. (11) is completely general. Generally, this equation can be used, e.g., to analyze the magnetic–field–induced change of gap parameter symmetry[27] or the upper critical field in the systems with the spin–triplet pairing. The latter area of application is especially attractive, since in these systems the Pauli pair breaking mechanism is absent, and the upper critical field is expected to be very high.[28]

III. RESULTS

A. Orbital effects

The transition lines $T_c(H)$, obtained in the absence of the Zeeman splitting ($g = 0$), are presented in Fig. 1.

Note that for a of the order of a few angströms, experimentally available magnetic fluxes are much less than Φ_0. Consequently, these plots correspond to the region of extremely high magnetic field. The size of the Hamiltonian matrix $H_{\mathbf{k}}$, that has to be diagonized for all values of $\mathbf{k}$ in each step of the iterative procedure, is $2q \times 2q$. Therefore, since the magnetic flux is proportional to q^{-1}, the proposed approach does not allow to carry out calculations for a small magnetic field. This is why the transition lines in Fig. 1. start at finite magnetic field.

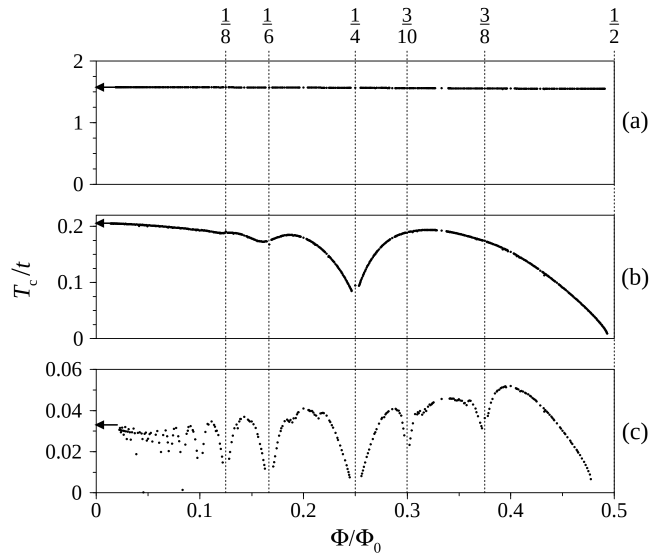

FIG. 1: Critical temperature T_c as a function of Φ/Φ_0. Upper, middle, and lower panel shows results for $V/t = 7$, 2 and 1, respectively. Small arrows indicate the transition temperature calculated from the usual BCS equations in the absence of magnetic field.

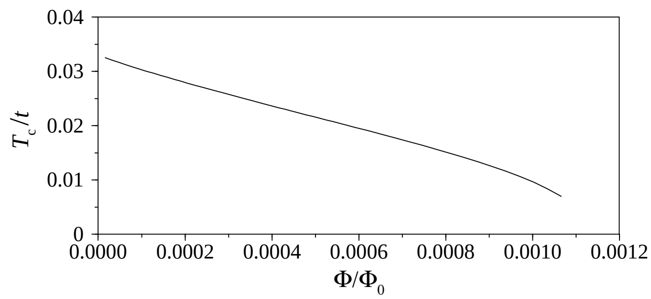

FIG. 2: Critical temperature T_c as a function of Φ/Φ_0 in the low field regime for $V/t = 1$. Results taken from Ref.[25]

For weak field thermal smearing and/or disorder induced broadening destroy the Hofstadter butterfly structure. In the absence of the lattice periodic potential this regime corresponds to a classical limit, where the number of occupied Landau levels is huge, and the Ginzburg–Landau description of the mixed state is valid. In this regime, in accordance with the common feeling, superconductivity in the tight–binding system is suppressed by magnetic field, disappearing at H_{c2}[25,29]. The corresponding transition line is presented in Fig. 2.

The method used in Ref.[25] does not work at low temperature and the present method does not work at weak

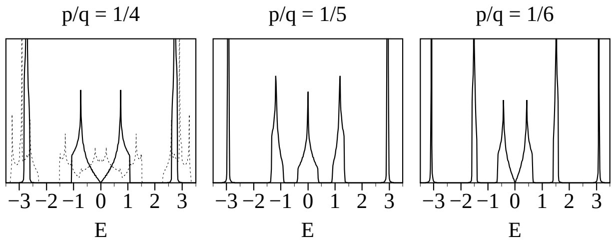

FIG. 3: Normal state density of states for different values of magnetic field. The dotted line in the first panel represents density of states in a superconducting state for different ratio p/q and for $\Delta = 0.7t$.

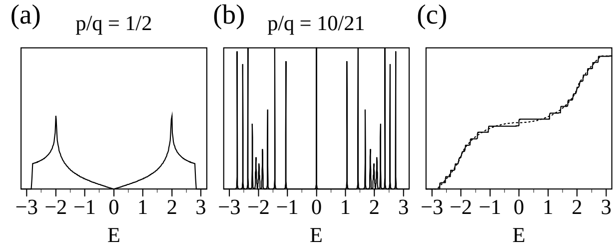

FIG. 4: Normal state density of states for $p/q = 1/2$ (a) and $p/q = 10/21$ (b). (c) Comparison of integrated densities of states for $p/q = 1/2$ (dotted line) and $p/q = 10/21$ (solid line).

field. Therefore, there is no crossover line from the low to high field regimes.

The transition lines for $1/2 < \Phi/\Phi_0 \leq 1$ can be obtained reflecting the lines presented in Fig. 1. around the line $\Phi/\Phi_0 = 1/2$, and $T_c(\Phi)$ is periodic on Φ_0. Both these properties reflect properties of the Hofstadter butterfly. Of course, these unphysical results are valid only when the Pauli pair breaking is neglected. The influence of the Zeeman splitting will be discussed later. For strong pairing potential, comparable with the band width, the critical temperature in the reentrant regime is almost field independent (see Fig 1a.). As V is reduced, the influence of the nontrivial density of states becomes apparent. It was shown by Hofstadter[9], that in normal state the Bloch band for $\Phi/\Phi_0 = p/q$ is symmetric and broken up into q distinct energy bands. In the half–filling case the Fermi level (E_F) is located in the center of the (unperturbed) subband. Therefore, if q is odd, F_E points to the singularity of the central subband (a remnant of the original van Hove singularity), whereas for even q it is in the gap between two subbands (In fact, for even q these subbands touch itself at the Fermi level). This is depicted in Fig. 3.

The changes of the density of states result in an oscillatory behavior of $T_c(H)$: T_c approaches its maxima for odd q and is reduced for even q. Similar oscillations were predicted by Rasolt and Tešanović[1] in a homogeneous system, where the Hofstadter spectrum is replaced by the Landau–level ladder.

The superconductivity suppression is especially apparent for small and even q, when V is comparable with the central–gap width. The smooth character of the function $T_c(\Phi)$ close to $\Phi/\Phi_0 = p/q$ and for small q (e.g., close to the values $p/q = 1/2,\ 1/3,\ 1/4$), seems counterintuitive, since a tiny detuning of the magnetic field completely changes the spectrum. For $p/q = 1/2$ the spectrum consists of two subbands, whereas for $p/q = 10/21$ there are 21 narrow subbands (see Fig.4). However, in spite of this difference, the integrated densities of states, presented in Fig. 4c, are almost the same.

For larger q, the differences between $1/q$ and $1/(q+1)$ are smaller, and consequently the distances between successive minima in the density of states decrease. For a strong pairing potential (and high T_c) there is large number of subbands within a range of energy $\sim k_B T_c$ and then the amplitude of oscillations is strongly reduced. On the other hand, for the weak potential (i.e., at low temperature), this irregular oscillations are visible even at low fields (cf. Fig. 1c).

B. Zeeman splitting

The previous discussion ignored the effect of Pauli pair breaking. We consider it next. Since the Zeeman splitting is proportional to the magnitude of the magnetic field and the orbital effect depends on the flux, we have to find a relation between these two quantities. It can be done by using the relation $t = \hbar^2/2m^*a^2$, where m^* is the effective mass. Then the Zeeman splitting is given by $g\mu_B H = 2\pi g^* \frac{p}{q} t$, where $g^* = g\frac{m^*}{m}$.[30]

The inclusion of the Zeeman term results in a reduction of the phase space available for pairing. For strong pairing potential, when the structure of the Hofstadter butterfly is hidden, it leads to a monotonic reduction of T_c with increasing magnetic field. Such a situation is presented in Fig. 5a.

However, for smaller values of V, when $k_B T_c$ is comparable with the miniband (or minigap) widths, the situation is more complicated. The Zeeman term leads to the splitting of each of the minibands into a spin–up and spin–down minibands. To have nonzero T_c we need minibands of both types present close to the Fermi level. As the magnitude of the splitting is proportional to the magnetic field, T_c will be an oscillatory function of the magnetic field. When the spin–up and spin–down minibands overlap at the Fermi level, T_c is strongly enhanced. This mechanism may induce superconductivity in regions, where T_c is zero or close to zero in the absence of the Zeeman splitting (compare the solid and dashed lines in Fig. 5b). For example, for $\Phi/\Phi_0 = 1/4$ E_F is located in the central minigap for $g^* = 0$, whereas there is a singularity at E_F for $g^* = 0.15$. The corresponding densities of states are presented in Fig. 6.

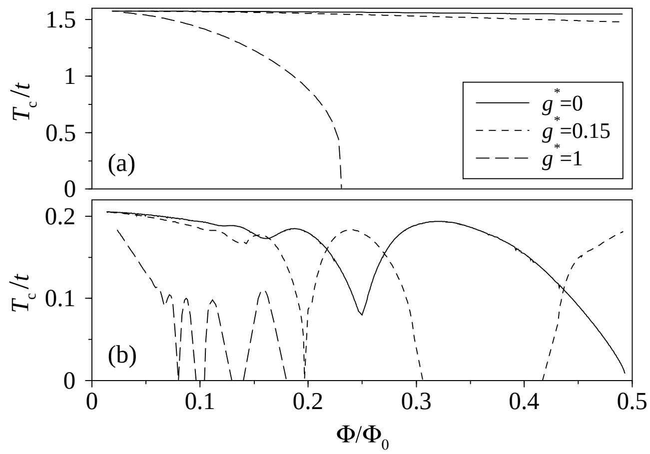

FIG. 5: Critical temperature T_c as a function of Φ/Φ_0 in the presence of the Zeeman splitting for $V/t = 7$ (a) and $V/t = 2$ (b).

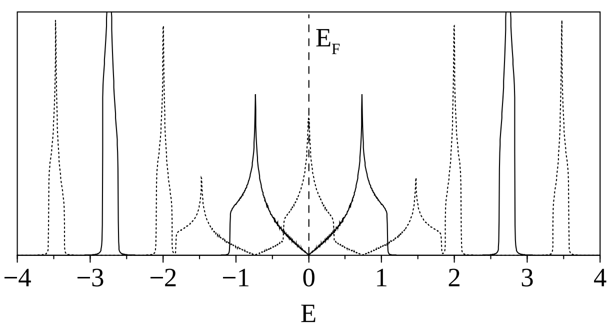

FIG. 6: Normal state densities of states for $\Phi/\Phi_0 = 1/4$. Solid and dashed lines correspond to $g^* = 0$ and $g^* = 0.15$, respectively.

IV. DISCUSSION

Let us comment on the possibility of observing the oscillatory behavior of T_c in real systems. Assuming lattice constant a=2Å the magnetic field required to obtain $\Phi/\Phi_0 \sim 1$ is $O(10^5)$T, which is obviously too large. However, there are some possibilities to overcome this problem. For example, it was recently shown[31], that in some three–dimensional systems fractal spectra, like Hofstadter's butterfly, can be obtained for $\Phi/\Phi_0 \ll 1$. On the other hand, it is possible to reach the needed increase of flux enlarging the lattice constant. Two–dimensional superconducting wire network can be suitable for this task, since the magnetic field corresponding to Φ_0 is about 1 mT for a network cell of 1 μm^2, and the system can be mapped onto a tight–binding one. Another possibility is connected with the case, where the influence of the modulation potential on the Landau–quantized 2D electron system may be considered as a small perturbation. This situation is complementary to the tight–binding case, but the energy spectrum is also obtained by solving the Harper equation. Therefore, one can expect similar behavior of T_c in 2D superconducting systems modulated in two dimensions. Again, since the modulation period is larger than the lattice constant, the required values of Φ are well within the experimental accessibility.

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